On the Numerical Solution of the Time Dependent Schrödinger Equation

R. Schäfer
University of Siegen, Fachbereich Physik, D-57068 Siegen, Germany,

R. Blendowske
Leica Mikroskopie und Systeme GmbH, D-35530 Wetzlar, Germany
(September 1994)

An algorithm for the numerical solution of the Schrödinger equation in the case of a time dependent potential is proposed. Our simple modification upgrades the well known method of Koonin while negligibly increasing the computing time. In the presented test the accuracy is enhanced by up to an order of magnitude.

02.60.+y, 25.85.-w

The microscopic description of many–body systems like atoms or nuclei is based on a many–body Hamiltonian. The related wave functions are given by Slater determinants for fermions. In the case of time dependent processes like atomic or nuclear collisions, nuclear fission or fusion, however, the situation is too complex due to the great number of degrees of freedom. Therefore, in most cases, a collective coordinate is introduced according to the essential physical properties of the considered system. This procedure leads to a macroscopic model with one degree of freedom, which is governed by an effective one–body Schrödinger equation including a time dependent potential in the considered examples [1]. The well known coordinate representation reads

$$i\hbar \, \frac{\partial}{\partial t} \, \phi \left(\mathbf{r}, t \right) = \left[-\frac{\hbar^2}{2 \, M} \, \nabla^2 \; + V \left(\mathbf{r}, t \right) \right] \; \phi \left(\mathbf{r}, t \right) \; . \tag{1}$$

A momentum dependent potential V, leading to an integro-differential equation, is excluded here. In almost all practical cases eq. (1) has to be evaluated numerically. The standard technique essentially consists of the following two steps: first apply a suitable scheme for the space discretization and then perform the time integration.

The algorithm presented here is only related to the second step: The time integration in the case of an explicitly time dependent potential $V(\mathbf{r}, t)$. Our proposed convenient modification upgrades the standard method to a much more efficient version while negligibly increasing the computing time.

Our experience is due to the description of ternary fission, i.e. a fission process accompanied by the emission of an α–particle, with results to be published elsewhere. However, the presented algorithm might be of broader interest, not necessarily restricted to this nuclear physics theme.

In this letter we will discuss the application for the case of a cylindrically symmetric, time dependent potential, essentially following Koonin's procedure [2], and present a test using an analytically solvable example.

As usual, in a cylindrically symmetric case, the angle dependence on φ of the wave function is separated as

$$\phi = \frac{1}{\sqrt{2\pi}} \; \psi(\rho, z, t) \; \exp(i\mu\varphi) \; , \tag{2}$$

and a grid is defined by

$$\begin{aligned} \rho_j &= (j - \frac{1}{2}) \; \Delta\rho \; , \quad j = 1, \ldots, N_\rho \; , \\ z_k &= k \; \Delta z \; , \quad k = -N_z, \ldots, N_z \; . \end{aligned} \tag{3}$$

For simplification we introduce now

$$g_{j,k} = \sqrt{\rho_j} \; \psi_{j,k} \tag{4}$$

leading to the space–discretized equation

$$i\hbar \, \frac{\partial}{\partial t} \, g_{j,k} = (Hg)_{j,k} = (vg)_{j,k} + (hg)_{j,k} \; , \tag{5}$$

where the Hamiltonian H is split in a "vertical" (v) and a "horizontal" (h) part

$$(vg)_{j,k} = -\frac{\hbar^2}{2M}\ \frac{c_j\ g_{j+1,k}\ -2\ g_{j,k}\ +c_{j-1}\ g_{j-1,k}}{\Delta\rho^{\,2}} +\ U_{j,k}\ g_{j,k}\ ,$$
$$(hg)_{j,k} = -\frac{\hbar^2}{2M}\ \frac{g_{j,k+1}\ -2\ g_{j,k}\ +\ g_{j,k-1}}{\Delta z^{\,2}} +\ U_{j,k}\ g_{j,k}\ , \tag{6}$$

with the abbreviations

$$c_j = \frac{j}{\sqrt{j^2-1/4}}\ ,$$
$$U_{j,k} = \frac{1}{2}V_{j,k} + \frac{\mu^2\hbar^2}{4M\rho_j^2}\ . \tag{7}$$

Up to this point no changes are made in comparison to Koonin's algorithm. We solve eq. (5) iteratively, with times $t_n = n\Delta t$, using a Taylor expansion of $g_{jk}(t_n) = g_{jk}^{(n)}$, up to and including $(\Delta t)^2$ and obtain

$$g^{(n+1)} = \Bigg(1 - \frac{i}{\hbar}\ H\ (\Delta t)^1$$
$$- \frac{1}{2\hbar^2}\ H^2\ (\Delta t)^2\ - \frac{i}{2\hbar}\ \dot{V}\ (\Delta t)^2 + \mathcal{O}\left(\Delta t^{\,3}\right)\Bigg)\quad g^{(n)}\ , \tag{8}$$

where all terms on the right hand side are evaluated at time t_n. The time derivative $\dot{V}_{j,k} = \partial V_{j,k}/\partial t$ is included to ensure consistency up to second order contributions.

Inserting $g^{(n)}$ on the right hand side is not an advisable method to determine $g^{(n+1)}$, because of serious numerical instabilities. Therefore, an "alternating direction implicit method" [3] is used, leading to a modified version of Koonin's algorithm

$$g^{(n+1)} = \left(1 + \frac{i}{2\hbar}\ v\ \Delta t + \frac{i}{8\hbar}\ \dot{V}\ (\Delta t)^2\ \right)^{-1}$$
$$\left(1 - \frac{i}{2\hbar}\ h\ \Delta t - \frac{i}{8\hbar}\ \dot{V}\ (\Delta t)^2\right)$$
$$\left(1 + \frac{i}{2\hbar}\ h\ \Delta t + \frac{i}{8\hbar}\ \dot{V}\ (\Delta t)^2\ \right)^{-1}$$
$$\left(1 - \frac{i}{2\hbar}\ v\ \Delta t - \frac{i}{8\hbar}\ \dot{V}\ (\Delta t)^2\right)\quad g^{(n)}\ , \tag{9}$$

where again all terms on the right hand side are evaluated at time t_n. Our result may be verified by an expansion in terms of Δt up to second order. There are no restrictions on the commutation of $[v, h]$. By neglecting terms dependent on $\dot{V}_{j,k}$, our expression reduces to the one used by Koonin et al. in [2].

For numerical convenience we now define $w^{(n)}$ by

$$\left(1 + \frac{i}{2\hbar}\ h\ \Delta t + \frac{i}{8\hbar}\ \dot{V}\ \ (\Delta t)^2\ \right)\ w^{(n)} = \left(1 - \frac{i}{2\hbar}\ v\ \Delta t - \frac{i}{8\hbar}\ \dot{V}\ (\Delta t)^2\ \right)\ g^{(n)} \tag{10}$$

leading to

$$\left(1 + \frac{i}{2\hbar}\ v\ \Delta t + \frac{i}{8\hbar}\ \dot{V}\ (\Delta t)^2\ \right)\ g^{(n+1)} = \left(1 - \frac{i}{2\hbar}\ h\ \Delta t - \frac{i}{8\hbar}\ \dot{V}\ (\Delta t)^2\ \right)\ w^{(n)}\ . \tag{11}$$

In order to determine $w^{(n)}$, and thereafter $g^{(n+1)}$, one has to invert tridiagonal matrices only, which can be performed by a suitable algorithm [4].

A central point for the efficiency of our modification is that the determination of

$$\dot{V}_{j,k}^{(n)} = \frac{V_{j,k}^{(n)} - V_{j,k}^{(n-1)}}{\Delta t} \tag{12}$$

up to order $(\Delta t)^0$ poses no appreciable effort. Anyway, the values of $V_{j,k}$ have to be calculated for all time steps in order to determine v and h. It is deemed unsuitable to compensate this by determining v and h at an intermediate

time step $t + \Delta t/2$ because one has to calculate the potential at this additional time step, as well. In many cases this produces appreciable effort. For example, in our calculations concerning the ternary fission it took approximately the same time to calculate $V^{(n)}$ for one value of n on the whole grid as to perform one iteration step from $g^{(n)}$ to $g^{(n+1)}$.

To test our algorithm, with regard to the modification due to keeping terms dependent on $\dot{V}$, we consider the following, explicitly time dependent potential

$$V\left(\mathbf{r},t\right) = \frac{1}{2}\, M\omega^2\, \mathbf{r}^{\,2} - 2\hbar\omega^2\, t\ . \tag{13}$$

At time $t = 0$ this is the potential of the harmonic oszillator with frequency ω. For the initial wave function we choose an eigenfunction of this harmonic oszillator

$$\phi\left(\mathbf{r}, t=0\right) = c_\ell\ H_\ell(\sqrt{\beta}\ z)\ \sqrt{\beta/\pi}\ \exp\left(-\frac{\beta}{2}\left[\rho^2 + z^2\right]\right)\ , \tag{14}$$

where $\beta = M\omega/\hbar$, $\ell \in \{0, 1, 2, \ldots\}$, H_ℓ = Hermite polynomial, and c_ℓ = constant of normalization.

The analytical solution is given by

$$\phi\left(\mathbf{r},t\right) = \phi\left(\mathbf{r}, t=0\right)\ \exp\left(-\,i\omega\left[\ell + 3/2\right] t + i\omega^2\, t^2\right)\ . \tag{15}$$

The results are displayed in Table I for different radial quantum numbers ℓ (different numbers of nodes of the wave function). Both parts of the wave function—real and imaginary—are considered separately. We use $\omega = 2$, $\Delta t = 1/60$ with 60 time steps and grid parameters $N_\rho = N_z = 64$ and $\Delta\rho = \Delta z = 0.25$. The enhancement in accuracy becomes as large as an order of magnitude. The norm of the wave function is (nearly) conserved, since the algorithm—modified or not—is nearly unitary [2].

We note that the considerations for a one dimensional time dependent potential are quite the same. One obtains

$$\begin{aligned}\phi\left(x, t+\Delta t\right) = &\left(\ 1 + \frac{i}{2\hbar}\, H\ \Delta t + \frac{i}{4\hbar}\, \dot{V}\ (\Delta t)^2\ \right)^{-1} \\ &\left(\ 1 - \frac{i}{2\hbar}\, H\ \Delta t - \frac{i}{4\hbar}\, \dot{V}\ (\Delta t)^2\ \right) \phi\left(x,t\right) + \mathcal{O}\ \left(\ \Delta t^{\,3}\ \right)\ .\end{aligned} \tag{16}$$

Again the calculation of $\dot{V}\left(x,t\right)$ poses nearly no effort. In contrast to the ordinary method, where the $\dot{V}$ terms are neglected [4], the above expression is accurate up to order $(\Delta t)^2$. The approximation (16) is unitary; it automatically maintains the normalization of ϕ. We note that no alternating direction method is needed in the one dimensional case.

We summarize: In the case of a time dependent potential the standard algorithm of Koonin can easily be modified to obtain a greater accuracy. Therefore, terms depending on $\dot{V}$ have to be included to get a consistent time expansion up to order $(\Delta t)^2$. The related algorithm has been shown to be superior in the presented numerical test.

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TABLE I. Results of the numerical test. The relative error of the real and imaginary part of the wave function is displayed for different numbers of nodes. The modification of the Koonin's standard algorithm lead to an enhancement in the accuracy of up to an order of magnitude.

nodes	Relative error of the real part:		Relative error of the imaginary part:	
	standard	modified	standard	modified
$\ell = 0$	10%	0.4%	4%	0.2%
$\ell = 1$	10%	0.6%	4%	0.4%
$\ell = 2$	1%	0.3%	40%	5%
$\ell = 3$	20%	4%	1.5%	0.6%